Hewlett Packard Enterprise

A COMPARISON OF GPU PROGRAMMING MODELS

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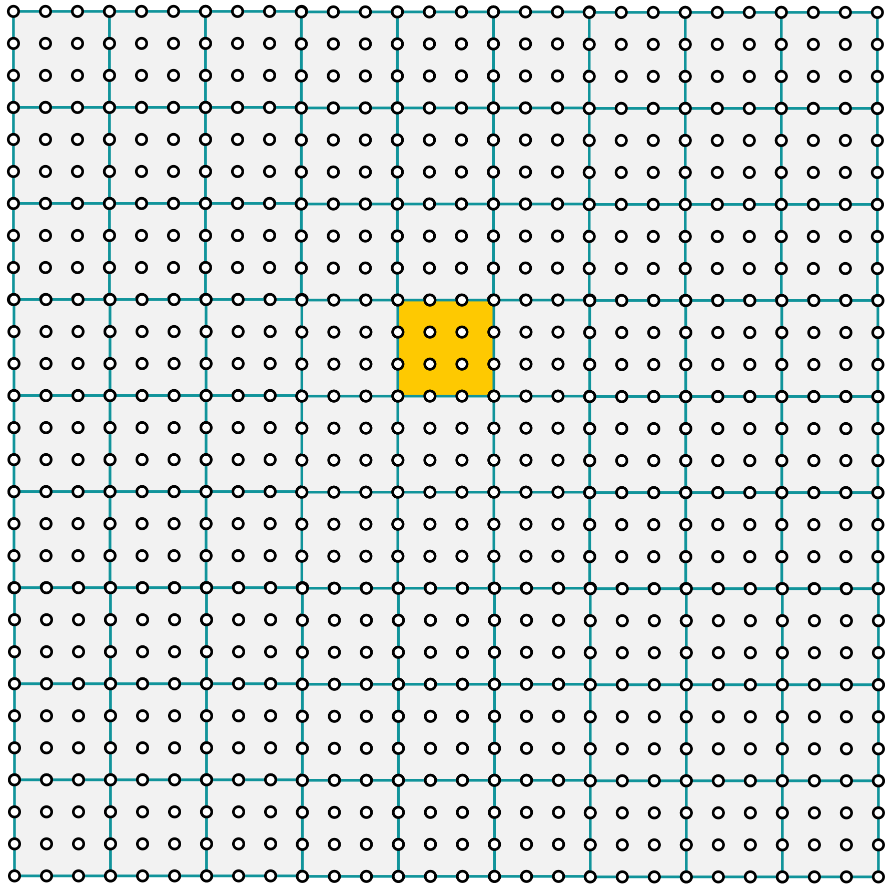
COMMUNICATION FROM NEKBONE BENCHMARK

- (3D) Grid of spectral elements
- That share faces that must be summed
- Partitioned across MPI tasks
- With contiguous buffers for MPI



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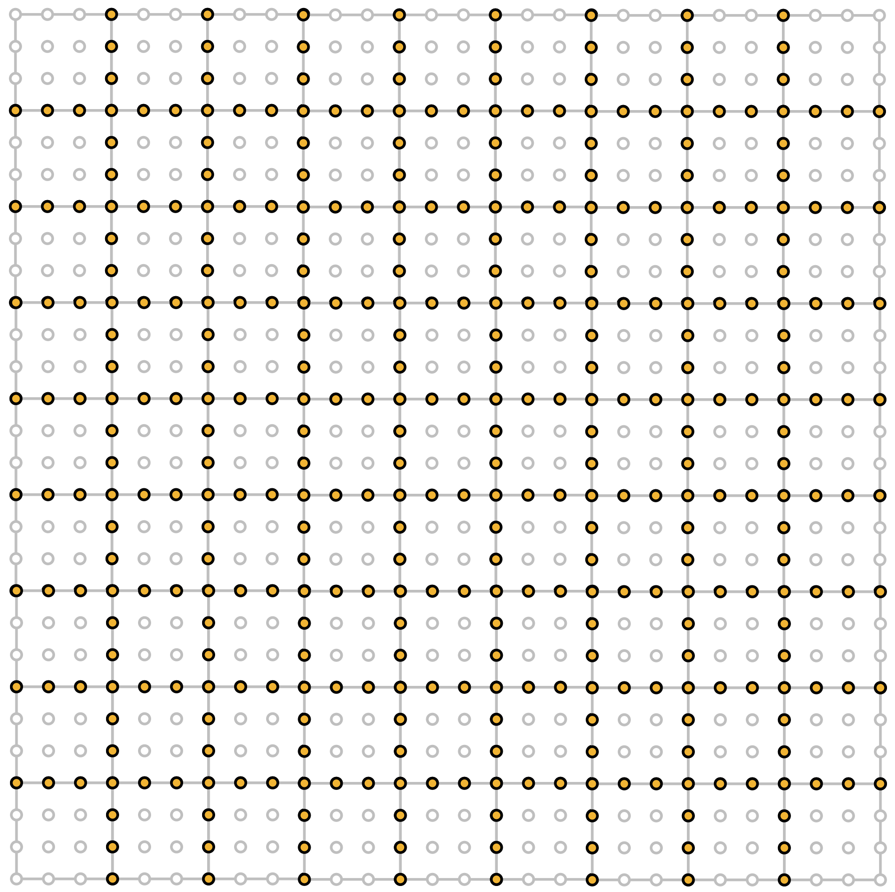

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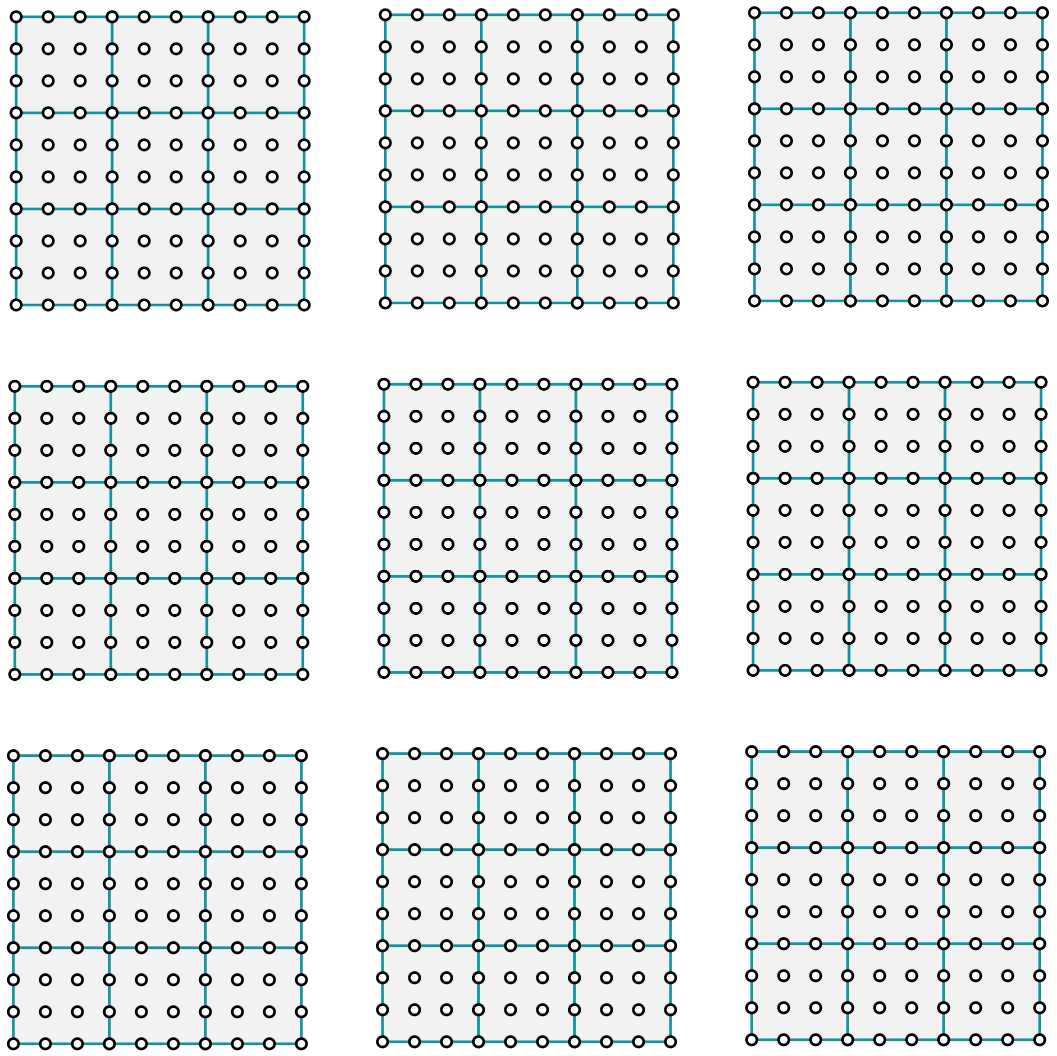

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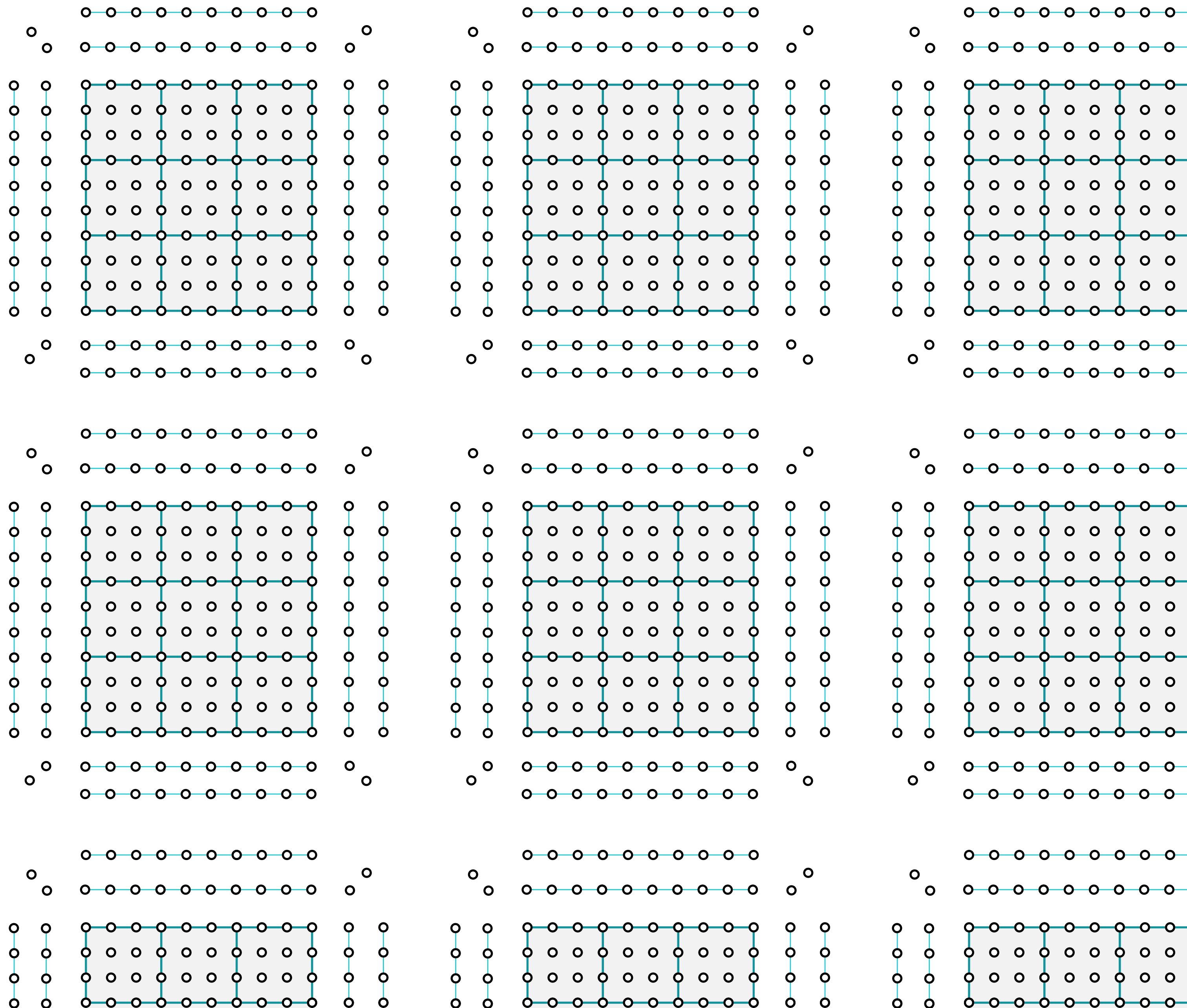
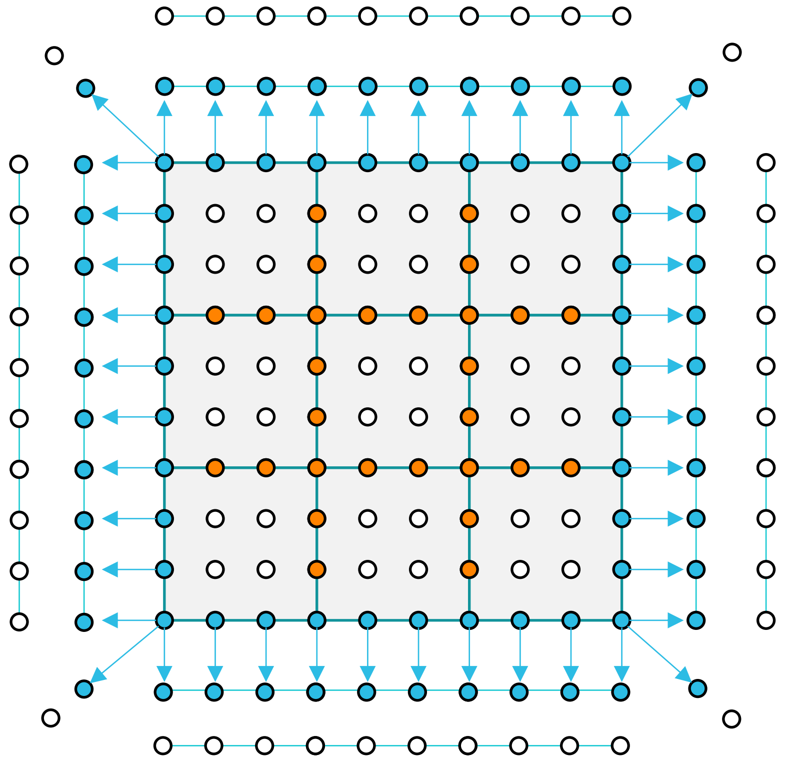


COMMUNICATION FROM NEKBONE BENCHMARK

- Overlap
  - Internal face sums
  - Copies into send buffers
  - MPI communication
  - Outer face **sums**



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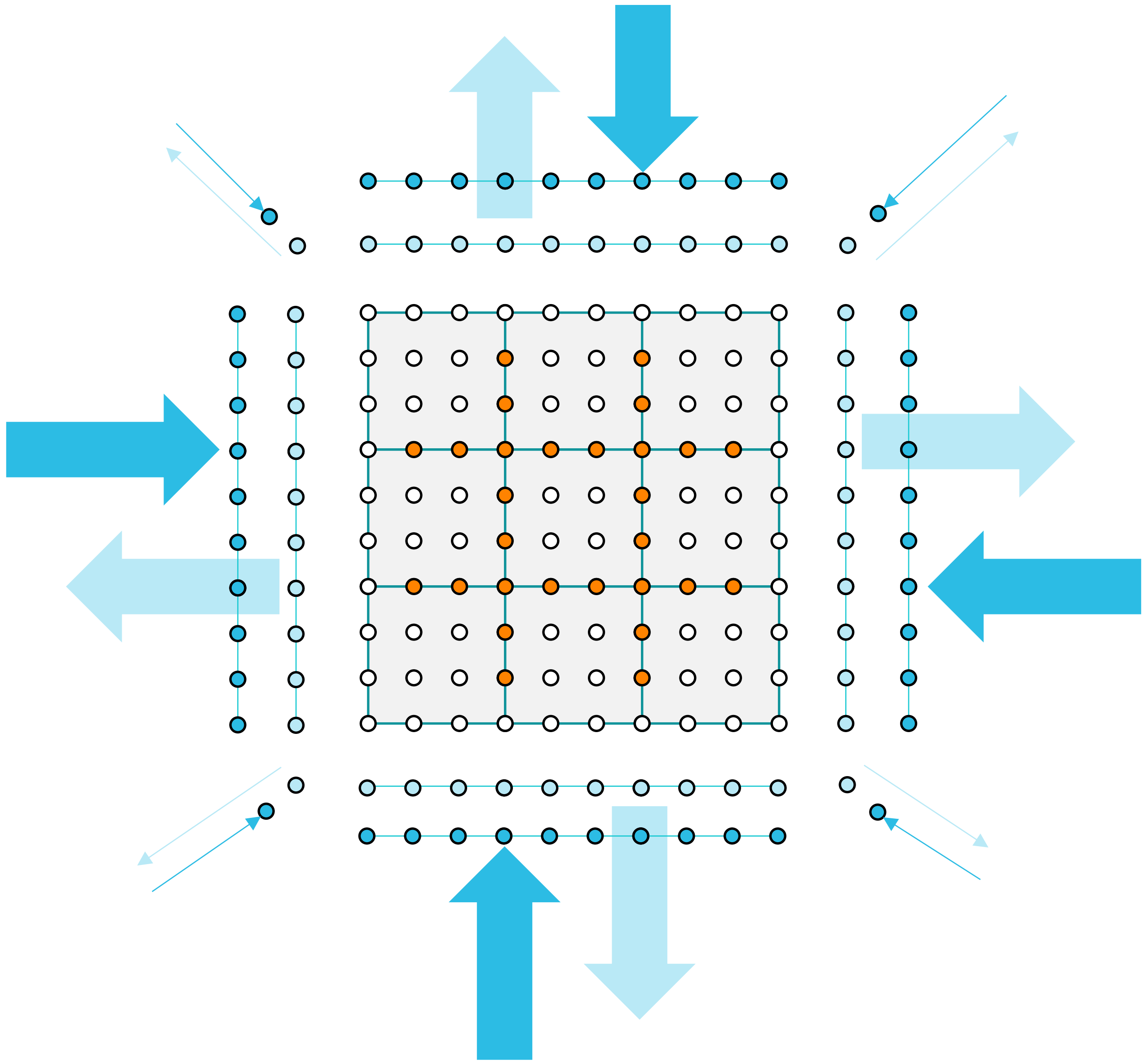

COMMUNICATION FROM NEKBONE BENCHMARK

- Overlap
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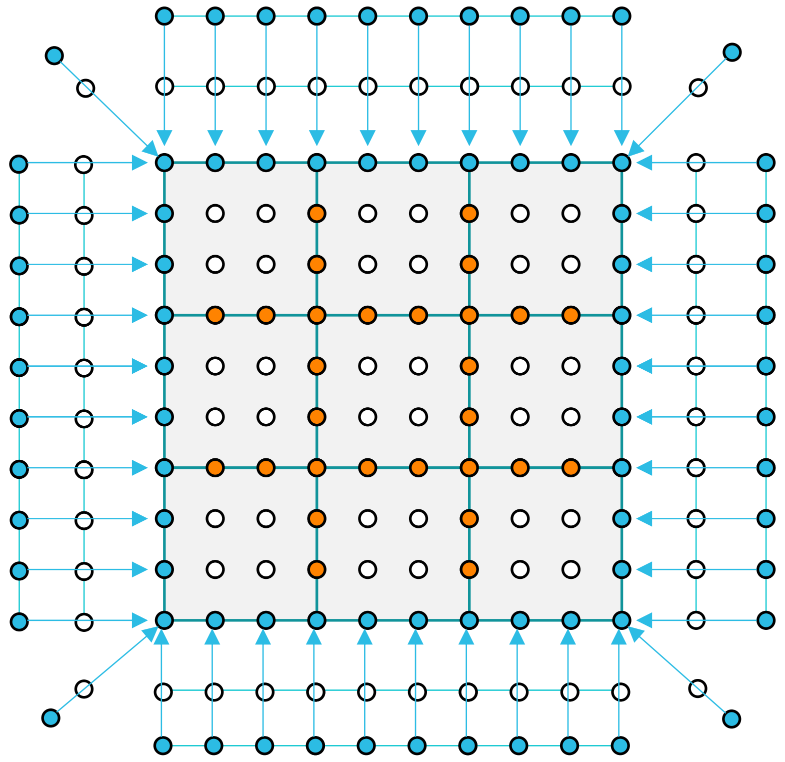

IMPLEMENTATIONS

- Fortran with OpenMP 4.5
- C++ with OpenMP 4.5
- C++ with Cuda
- C++ with Hip
- C++ with Kokkos
- C++ with Raja and Umpire

FEATURE COMPARISON

- Multi-dimensional arrays
- Elements stored on GPUs
- MPI buffers stored on GPUs
- Translating loops to kernels
- Running kernels in parallel

FEATURE COMPARISON

- **Multi-dimensional arrays**
- Elements stored on GPUs
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MULTI-DIMENSIONAL ARRAYS

- Fortran with OpenMP: **native**
- C++ with OpenMP
  - **Current implementations don't map objects effectively**
  - Forces C-like code
  - Cannot yet port existing array classes
- Cuda and Hip
  - Do it yourself
  - Good support for C++ modularity features:
    constructors, destructors, operator overloading, lambdas
  - **Port existing array classes**

MULTI-DIMENSIONAL ARRAYS

- **`Kokkos::View`**
  - Defaults to column major for GPUs
  - Owns memory, includes copy methods
  - Intended to replace existing array classes?
- **`RAJA::View`**
  - Defaults to row major
  - Wraps a provided pointer
  - Can use Umpire to allocate and copy
  - Not a stand-alone array class
  - Useful for porting existing array classes

FEATURE COMPARISON

- Multi-dimensional arrays
- **Elements stored on GPUs**
- MPI buffers stored on GPUs
- Translating loops to kernels
- Running kernels in parallel

ELEMENTS STORED ON GPUS: FORTRAN WITH OPENMP

- Map clauses (no need for array dimensions)

```
!$omp target data map(u)
...
!$omp end target data
```

- Eliminate implicit copies by enclosing larger regions in `target data`
- Nest `target data` regions, may be lower in call stack
- Allows incremental tuning and debugging
- **WARNING:** Changes in caller code can change local OpenMP semantics

ELEMENTS STORED ON GPUS: C++ WITH OPENMP

- Current implementations of **`map`** clauses have limitations
- Support for raw pointers only, not array classes
- Need explicit array bounds
- Need local copies of **`this`** member variables

```
// `du_` and `ue_` are member variables
// Make local copies
int *const du = du_;
double *const ue = ue_;
#pragma omp target data map(to:du[:6]) map(ue[:du[5]])
```

ELEMENTS STORED ON GPUS

- **`Kokkos::View`**
  - On GPU by default
  - Can create explicitly host-allocated **`Kokkos::View`**
  - Supports explicit copies between GPU and host views
- Cuda, Hip, Raja
  - Allocate GPU memory
  - Do explicit copies to/from host pointers
  - Raja: Can use Umpire to avoid GPU-specific code

FEATURE COMPARISON

- Multi-dimensional arrays
- Elements stored on GPUs
- **MPI buffers stored on GPUs**
- Translating loops to kernels
- Running kernels in parallel

MPI BUFFERS STORED ON GPUS: FORTRAN WITH OPENMP

- MPI buffers can be module variables
- Init procedure allocates them on GPU, deallocating first if necessary

```
!$omp taskwait
if (initted_) then
  !$omp target exit data map(delete:corner_)
  ! deallocate host arrays
  ...
end if
initted_ = .true.
! allocate and initialize host arrays
...
!$omp target enter data map(to:corner_)
...
```

MPI BUFFERS STORED ON GPUS: C++ WITH OPENMP

- MPI buffers can be class members
- Constructor maps **`to`**, destructor maps **`delete`**

```
Faces::Faces(...):
  ...
  xfr0_(nullptr),xfr1_(nullptr)
{
  ...
  alloc(xfr0_,dxf_[3]);
  alloc(xfr1_,dxf_[3]);
  ...
```

```
static void alloc(double *&p, const long n)
{
  double *const q = new double[n];
  memset(q,0,n*sizeof(double));
  #pragma omp target enter data map(to:q[:n])
  p = q;
}
```

MPI BUFFERS STORED ON GPUS: FORTRAN AND C++ WITH OPENMP

- MPI access to GPU pointers through **`use_device_ptr`**

```
!$omp target data map(u) &
!$omp use_device_ptr(xface_,yface_,zface_,xedge_,yedge_,zedge_,corner_)
...
```

```
#pragma omp target data use_device_ptr(xfr0,xfr1,yfr0,yfr1,zfr0,zfr1)
{
  MPI_Irecv(xfr0,dxf_[3],MPI_DOUBLE,iface_[0],tag,MPI_COMM_WORLD,reqr_+0);
  MPI_Irecv(xfr1,dxf_[3],MPI_DOUBLE,iface_[1],tag,MPI_COMM_WORLD,reqr_+1);
  MPI_Irecv(yfr0,dyf_[3],MPI_DOUBLE,iface_[2],tag,MPI_COMM_WORLD,reqr_+2);
  MPI_Irecv(yfr1,dyf_[3],MPI_DOUBLE,iface_[3],tag,MPI_COMM_WORLD,reqr_+3);
  MPI_Irecv(zfr0,dzf_[3],MPI_DOUBLE,iface_[4],tag,MPI_COMM_WORLD,reqr_+4);
  MPI_Irecv(zfr1,dzf_[3],MPI_DOUBLE,iface_[5],tag,MPI_COMM_WORLD,reqr_+5);
}
```

MPI BUFFERS STORED ON GPUS: CUDA, HIP, KOKKOS, RAJA

- Contiguous MPI buffers are on GPU
- Array objects return raw GPU pointer
- MPI uses GPU pointers directly

```
MPI_Isend(xes0.data(),nedge_[0],MPI_DOUBLE,iedge_[0],tag,
          MPI_COMM_WORLD,reqs_+6);
```

FEATURE COMPARISON

- Multi-dimensional arrays
- Elements stored on GPUs
- MPI buffers stored on GPUs
- **Translating loops to kernels**
- Running kernels in parallel

TRANSLATING LOOPS TO KERNELS

- Fortran with OpenMP
  - Easy! For **N** nested loops:
    `!$omp target teams distribute parallel do simd collapse(N)`
  - Cray Fortran compiler just needs **`distribute`**, others look for **`parallel do`**
- C++ with OpenMP
  - Easy! For **N** nested loops:
    `#pragma omp target teams distribute parallel for simd collapse(N)`
  - Implementations pretty much agree on emphasizing **`parallel for`**
- Cuda, Hip
  - Do it yourself

TRANSLATING LOOPS TO KERNELS: KOKKOS

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: KOKKOS

default target set at build time
asynchronous with host by default

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: KOKKOS

string name for Kokkos' built-in profiling

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: KOKKOS

triply nested loops

automatic mapping of loops to hardware

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: KOKKOS

loop body as lambda

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: KOKKOS

`Kokkos::View` ***operators***

```
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>({1,1,1},{mx,my,mz}),
KOKKOS_LAMBDA(const int jx, const int jy, const int jz) {
  u(0,0,0,jx,jy,jz) += u(nm1,0,0,jx-1,jy,jz)
    +u(0,nm1,0,jx,jy-1,jz)+u(nm1,nm1,0,jx-1,jy-1,jz)
    +u(0,0,nm1,jx,jy,jz-1)+u(nm1,0,nm1,jx-1,jy,jz-1)
    +u(0,nm1,nm1,jx,jy-1,jz-1)+u(nm1,nm1,nm1,jx-1,jy-1,jz-1);
  u(nm1,0,0,jx-1,jy,jz) = u(0,nm1,0,jx,jy-1,jz)
    = u(nm1,nm1,0,jx-1,jy-1,jz) = u(0,0,nm1,jx,jy,jz-1)
    = u(nm1,0,nm1,jx-1,jy,jz-1) = u(0,nm1,nm1,jx,jy-1,jz-1)
    = u(nm1,nm1,nm1,jx-1,jy-1,jz-1) = u(0,0,0,jx,jy,jz);
});
```

TRANSLATING LOOPS TO KERNELS: RAJA

similar to Kokkos

body in lambda

`RAJA::View` ***operators***

```
RAJA::kernel<for3async>(
  RAJA::make_tuple(r1mx,r1my,r1mz),
  [=] RAJA_DEVICE (const int jx, const int jy, const int jz) {
    u(jz,jy,jx,0,0,0) += u(jz,jy,jx-1,0,0,nm1)
      +u(jz,jy-1,jx,0,nm1,0)+u(jz,jy-1,jx-1,0,nm1,nm1)
      +u(jz-1,jy,jx,nm1,0,0)+u(jz-1,jy,jx-1,nm1,0,nm1)
      +u(jz-1,jy-1,jx,nm1,nm1,0)+u(jz-1,jy-1,jx-1,nm1,nm1,nm1);
    u(jz,jy,jx-1,0,0,nm1) = u(jz,jy-1,jx,0,nm1,0)
      = u(jz,jy-1,jx-1,0,nm1,nm1) = u(jz-1,jy,jx,nm1,0,0)
      = u(jz-1,jy,jx-1,nm1,0,nm1) = u(jz-1,jy-1,jx,nm1,nm1,0)
      = u(jz-1,jy-1,jx-1,nm1,nm1,nm1) = u(jz,jy,jx,0,0,0);
  });
```

TRANSLATING LOOPS TO KERNELS: RAJA

execution policy and ranges defined in user code and reused

```
RAJA::kernel<for3async>(
  RAJA::make_tuple(r1mx,r1my,r1mz),
  [=] RAJA_DEVICE (const int jx, const int jy, const int jz) {
    u(jz,jy,jx,0,0,0) += u(jz,jy,jx-1,0,0,nm1)
      +u(jz,jy-1,jx,0,nm1,0)+u(jz,jy-1,jx-1,0,nm1,nm1)
      +u(jz-1,jy,jx,nm1,0,0)+u(jz-1,jy,jx-1,nm1,0,nm1)
      +u(jz-1,jy-1,jx,nm1,nm1,0)+u(jz-1,jy-1,jx-1,nm1,nm1,nm1);
    u(jz,jy,jx-1,0,0,nm1) = u(jz,jy-1,jx,0,nm1,0)
      = u(jz,jy-1,jx-1,0,nm1,nm1) = u(jz-1,jy,jx,nm1,0,0)
      = u(jz-1,jy,jx-1,nm1,0,nm1) = u(jz-1,jy-1,jx,nm1,nm1,0)
      = u(jz-1,jy-1,jx-1,nm1,nm1,nm1) = u(jz,jy,jx,0,0,0);
  });
```

TRANSLATING LOOPS TO KERNELS: RAJA

execution policy and ranges defined in user code and reused

```
// in header
using for3async = RAJA::KernelPolicy<GPU_KERNEL_ASYNC<
   RAJA::statement::For<2,GPU_BLOCK_Y_LOOP,
   RAJA::statement::For<1,GPU_BLOCK_X_LOOP,
   RAJA::statement::For<0,GPU_THREAD_X_LOOP,
   RAJA::statement::Lambda<0>>>>>>;

// in caller
const RAJA::RangeSegment r1mx(1,mx_);
const RAJA::RangeSegment r1my(1,my_);
const RAJA::RangeSegment r1mz(1,mz_);
```

TRANSLATING LOOPS TO KERNELS: RAJA

explicit mapping of loops to implementation

```
// in header
using for3async = RAJA::KernelPolicy<GPU_KERNEL_ASYNC<
   RAJA::statement::For<2,GPU_BLOCK_Y_LOOP,
   RAJA::statement::For<1,GPU_BLOCK_X_LOOP,
   RAJA::statement::For<0,GPU_THREAD_X_LOOP,
   RAJA::statement::Lambda<0>>>>>>;

// in caller
const RAJA::RangeSegment r1mx(1,mx_);
const RAJA::RangeSegment r1my(1,my_);
const RAJA::RangeSegment r1mz(1,mz_);
```

TRANSLATING LOOPS TO KERNELS: RAJA

***GPU portability through* `#ifdefs`**

```
// in header
using for3async = RAJA::KernelPolicy<GPU_KERNEL_ASYNC<
   RAJA::statement::For<2,GPU_BLOCK_Y_LOOP,
   RAJA::statement::For<1,GPU_BLOCK_X_LOOP,
   RAJA::statement::For<0,GPU_THREAD_X_LOOP,
   RAJA::statement::Lambda<0>>>>>>;

// in caller
const RAJA::RangeSegment r1mx(1,mx_);
const RAJA::RangeSegment r1my(1,my_);
const RAJA::RangeSegment r1mz(1,mz_);
```

TRANSLATING LOOPS TO KERNELS: RAJA

GPU portability through **`#ifdefs`**

```
#ifdef RAJA_ENABLE_HIP
#define GPU_BLOCK_X_LOOP RAJA::hip_block_x_loop
#define GPU_BLOCK_Y_LOOP RAJA::hip_block_y_loop
#define GPU_BLOCK_Z_LOOP RAJA::hip_block_z_loop
#define GPU_KERNEL_ASYNC RAJA::statement::HipKernelAsync
...
#elif defined RAJA_ENABLE_CUDA
#define GPU_BLOCK_X_LOOP RAJA::cuda_block_x_loop
#define GPU_BLOCK_Y_LOOP RAJA::cuda_block_y_loop
#define GPU_BLOCK_Z_LOOP RAJA::cuda_block_z_loop
#define GPU_KERNEL_ASYNC RAJA::statement::CudaKernelAsync
...
#endif
```

FEATURE COMPARISON

- Multi-dimensional arrays
- Elements stored on GPUs
- MPI buffers stored on GPUs
- Translating loops to kernels
- **Running kernels in parallel**

RUNNING KERNELS IN PARALLEL

- Running multiple kernels at the same time on a single GPU (while running asynchronously with host)
- Cuda, Hip: launch kernels on different streams
- OpenMP

```
!$omp target team depend(out:xface_) nowait
#pragma omp target teams depend(out:xfs0) nowait
```

  - Don't try to identify all actual variable dependencies
  - Think of **`depend`** target as virtual stream identifier
  - Like a table translates variable addresses to GPU streams
- Raja: no explicit support yet

RUNNING KERNELS IN PARALLEL: KOKKOS

Construct execution spaces associated with different GPU streams (can be class member variables)

```
Kokkos::DefaultExecutionSpace inner(innerStream);
Kokkos::DefaultExecutionSpace outer(outerStream);
...
Kokkos::parallel_for("faces",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>(outer,{0,0,0},{n,n,mm}),
  ...
});
...
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>(inner,{1,1,1},{mx,my,mz}),
  ...
});
```

RUNNING KERNELS IN PARALLEL: KOKKOS

```
Kokkos::DefaultExecutionSpace inner(innerStream);
Kokkos::DefaultExecutionSpace outer(outerStream);
...
Kokkos::parallel_for("faces",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>(outer,{0,0,0},{n,n,mm}),
   ...
});
...
Kokkos::parallel_for("internal corners",
Kokkos::MDRangePolicy<Kokkos::Rank<3>>(inner,{1,1,1},{mx,my,mz}),
   ...
});
```

Kernels launched with different execution spaces can run concurrently on the same GPU

FEATURE COMPARISON

- Multi-dimensional arrays
- Elements stored on GPUs
- MPI buffers stored on GPUs
- Translating loops to kernels
- Running kernels in parallel

OTHER TOPICS TO CONSIDER

- Mapping MPI tasks to GPUs
- Fusing kernel launches
- GPU synchronization for MPI sends
- Translating loops to Cuda and Hip kernels
- Shmem communication inside kernels

EXTERNAL LINKS

- Coral-2 Benchmarks (home of Nekbone benchmark): https://asc.llnl.gov/coral-2-benchmarks/
- OpenMP Specifications: https://www.openmp.org/specifications/
- Cuda Toolkit Documentation: https://docs.nvidia.com/cuda/
- Hip Programming Guide: https://rocmdocs.amd.com/en/latest/Programming_Guides/HIP-GUIDE.html
- The Kokkos Lectures: https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series
- Raja User Guide: https://raja.readthedocs.io/en/main/
- Umpire documentation: https://umpire.readthedocs.io/en/develop/index.html

THANK YOU

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